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Tunneling Effects On Low Energy Fusion Cross Sections (U)

September 1989   Authors:
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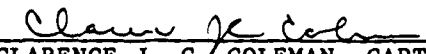California 93523-5000

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FOREWORD

This final report was submitted Christopher L. Leakeas, Purdue University, on completion of this special task with the Astronautics Laboratory (AFSC), Edwards Air Force Base CA. The AL Project Manager was Dr Franklin B. Mead, Jr.

This report has been reviewed and is approved for release and distribution in accordance with the distribution statement on the cover and on the DD Form 1473.

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Deputy Director, Astronautical Sciences
  Division

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Recently, the claim of discovery of "cold fusion" among the isotopes of hydrogen in a metal lattice has raised many questions as to the cross sections of some fusion reactions at low energies. This report investigates the quantum phenomenon of tunneling and its effects on the fusion process. Special attention is paid to penetrabilities in the Hulthen potential, which gives a reasonably accurate approximation of the potential inside the metal lattice. This report includes cross section data for the DD, DT amd pD reactions. Also given are graphs showing the fusion cross section crossover point between the DD and DT reactions and the increased penetrabilities due to enhanced tunneling effects.

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INTRODUCTION

One of the most promising technologies in the world today is nuclear fusion. Fusion could someday provide a cheap, relatively clean source of energy to meet the world's growing energy demands, but many problems must still be solved before fusion can become a commercially viable source of energy.

Nuclear fusion is the means by which two ions (typically low atomic number) collide and momentarily stick together, forming an excited nucleus, which then breaks apart into reaction products with a resulting net decrease in mass. This "mass deficit" is converted into the kinetic energy of the reaction products according to Einstein's equation $E = mc^2$. The energy of these products can then be converted into electricity either by direct energy conversion for charged particles or by converting their kinetic energy to heat a working fluid to drive a thermodynamic cycle for uncharged particles, like neutrons.

BARRIER PENETRATION

Since like charges repel when they approach one another, there is a problem getting ions close enough for a fusion reaction to occur. If the ions can be brought to within about 50 fm (approximately the nuclear radius) the short-range strong nuclear force dominates the weaker Coulomb repulsion and pulls the ions together. The problem lies in giving the ions enough energy to overcome the repulsive force.

Classically, the ions must have more energy than the height of the Coulomb barrier (which varies as the product of the nuclear charges of the reacting ions) at the nuclear radius in order to react. That means that in order for two Z=1 ions to come close enough to fuse, each ion must have approximately 288 keV of energy. If each ion in a thermonuclear plasma had this energy, the temperature of the plasma would be over three trillion degrees Kelvin. Heating and containing such high energy plasmas is far beyond the realm of technology today. However, because of a quantum mechanical effect known as "tunneling" or "barrier penetration" such temperatures are not necessary. Since thermonuclear plasmas are not monoenergetic but have very broad energy distributions, there are always

particles that have enough energy to overcome the Coulomb barrier. In plasmas attainable by today's technologies, a vast majority of particles still aren't energetic enough. This is the reason that tunneling plays an important role in the fusion process.

Classically, if a particle approaches a Coulomb barrier, it will be decelerated until it is stopped and then accelerated in the opposite direction. In quantum mechanics there exists a finite probability that two colliding particles will react. To describe this phenomena in a physically meaningful way, we must introduce the concept of wave function. It is no longer appropriate to talk about particles as being extended masses with a definite momentum and position. Rather, we must talk of a possible spread range of momenta and a probability of finding the "particle" at a certain point in space based on the "Heisenberg Uncertainty Principle" (Ref. 1). Heisenberg's principle sets a lower limit on the product of the uncertainties in momentum and position.

$$\Delta p_x \Delta x \geq \hbar \qquad (1)$$

where $\hbar = h/2\pi$ and h is Planck's constant, 6.626×10^{-34} J·s. The square of the wave function represents the probability amplitude, that is, the probability of finding the particle at any point in space at any time. The wave function, $U(\vec{r}, t)$, is found by solving Schrödinger's equation:

$$\frac{-\hbar^2}{2M} \nabla^2 U(\vec{r}, t) + V(\vec{r}) U(\vec{r}, t) = i\hbar \frac{\partial U(\vec{r}, t)}{\partial t} \qquad (2)$$

subject to certain boundary conditions (usually that the wave function and its first derivative be continuous). Treating this as a one dimensional problem and separating out the time dependence using separation of variables, we are left with the one dimensional, time-independent Schrodinger's equation given by

$$HU = EU \qquad (3)$$

where H is the Hamiltonian operator $(p^2/2M + V(x))$ and E is the eigenvalue of the Hamiltonian. This can also be written as

$$\frac{-\hbar^2}{2M} \frac{d^2 U}{dx^2} + V(x) U = EU \qquad (4)$$

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Solving for the second derivitive and multiplying by $2\frac{dU}{dx}$

we are left with

$$\frac{d}{dx}\left(\frac{dU}{dx}\right)^2 = \frac{4M}{\hbar^2}\frac{dU}{dx}[V(x) - E]U \tag{5}$$

integrating twice (to get U(x)) and squaring gives us the probability amplitude, or the barrier penetration factor, B

$$B = \exp\left[-2\int_{0}^{x_0}\left\{\frac{2M}{h^2}[V(x) - E]\right\}^{1/2}dx\right] \tag{6}$$

where x_0 is the point at which the particle would be turned around if a classical treatment of the problem was used. Using a classical treatment of the problem, a particle cannot enter a region of space where its potential energy would be greater than its initial kinetic energy. By analogy, a ball cannot roll up a hill any farther than a point where the ball's gravitational potential energy equals its initial kinetic energy. This makes the region between the point of closest approach (the turning point) and the nucleus a classically forbidden region, which means that there is zero probability of finding the particle there at any instant in time. However, by solving the Schrodinger equation we have shown that the wave function, and therefore the probability, is not zero beyond the turning point but decays exponentially across this classically forbidden region. Therefore, there is a finite probability of the two ions tunneling through their mutual Coulomb repulsive barrier and fusing because of the much stronger nuclear force. This probability depends on the height of the barrier, V(r), the thickness of the barrier, $r_0 - r_n$ (where r_n is the nuclear radius), the reduced mass of the two particle system, and the relative energy of the particles in Equations 7-10 (Ref. 1).

height $\quad V(r) = \frac{Z_1 Z_2 e^2}{r}$ \hfill (7)

thickness $\quad t = \frac{Z_1 Z_2}{E} - r_n$ \hfill (8)

reduced mass $\quad M = \frac{m_1 m_2}{m_1 + m_2}$ \hfill (9)
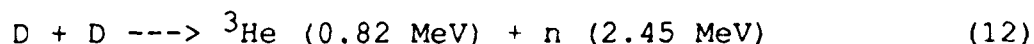
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CM energy $\qquad E = 0.5Mv^2$ (10)

   If the particles approach with a high relative energy, there is very little of the barrier to tunnel through. Although the probability of finding the particle inside the barrier drops off exponentially, there still remains a "good" probability of the particles reacting. On the other hand, if the particles approach each other with a low relative energy, the barrier is both high and wide and there is very little chance of tunneling. This is the concept behind thermonuclear fusion. Plasmas are heated to very high temperatures, (the necessary temperatures vary as the reaction products change) to reach ignition and start the fusion process. Ignition is defined as the point at which the power gained is equal to the power lost by the reactor due to conduction loss, particle loss, and radiative losses (such as cyclotron and Bremsstrahlung) (Ref. 3). At this point, the reaction is self-sustaining because some of the highly energetic charged reaction products give up a portion of their energy to the ions in the plasma, which keeps the plasma temperature above the ignition temperature, therefore, high enough to sustain the reaction.
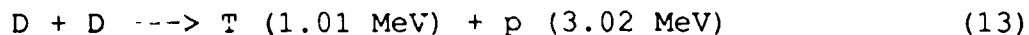
   Since the tunneling probability decays exponentially as the product of the charges and the reduced mass increase, it is apparent that the tunneling probabilities are greatest between isotopes of hydrogen. In fact, the main fusion reaction being studied today (because of its relatively low ideal ignition temperature, 3.5 keV) is between deuterons (^{2}H nuclei) and tritons (^{3}H nuclei) (Ref. 4). This reaction proceeds according to :

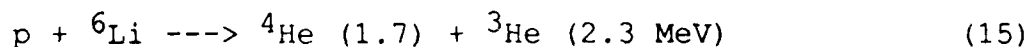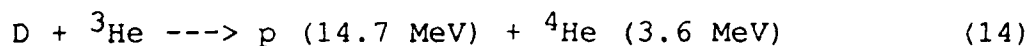$$D + T \longrightarrow {}^4He\ (3.52MeV) + n\ (14.1\ MeV)$$ (11)
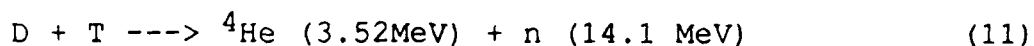
   This is not a desirable reaction since most of the energy is carried by the neutron which is harder to convert to usable energy. Another negative consequence of neutron production is the heavy shielding which would be required. Over a period of time, large neutron fluxes could cause radiation damage to the reactor's first wall causing the wall to become brittle, or to make the shielding radioactive creating a disposal problem.

   Another likely reaction is between two deuterons. This reaction proceeds by two branches, each with about the same probability.

$$D + D \longrightarrow {}^3He\ (0.82\ MeV) + n\ (2.45\ MeV)$$ (12)

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$$D + D \longrightarrow T \ (1.01 \ \text{MeV}) + p \ (3.02 \ \text{MeV}) \tag{13}$$

Again, not a very desirable reaction since much of the energy is carried away by neutrons. Some aneutronic reactions are :

$$D + {}^3\text{He} \longrightarrow p \ (14.7 \ \text{MeV}) + {}^4\text{He} \ (3.6 \ \text{MeV}) \tag{14}$$

$$p + {}^6\text{Li} \longrightarrow {}^4\text{He} \ (1.7) + {}^3\text{He} \ (2.3 \ \text{MeV}) \tag{15}$$

$$p + {}^{11}\text{B} \longrightarrow 3 \ {}^4\text{He} \ (2.89 \ \text{MeV each}) \tag{16}$$

$${}^3\text{He} + {}^3\text{He} \longrightarrow 2p \ (5.7 \ \text{MeV each}) + {}^4\text{He} \ (1.43 \ \text{MeV}) + \tag{17}$$

These reactions involve at least one reactant with $Z>1$, so the tunneling effect is not as great. Most of these reactions have very high ignition temperatures and are referred to as "advanced fuel reactions".

COLD FUSION

Recently, much attention has focused on the University of Utah where Drs. Pons and Fleischmann have reported seeing great amounts of heat produced by forcing excess amounts of deuterium into a metal lattice. They claim that this excess heat can only be explained as the result of "solid state" or "cold" nuclear fusion between deuterons occupying the same sites in a palladium lattice. Since Pons and Fleischmann have been very discrete with details of their experimental process pending decisions on their patent applications, no one is exactly sure of their experimental method. Many researchers have tried to duplicate their results with only limited success. If indeed this is the fusion of deuterons, there should be evidence of neutrons, tritium, and helium being evolved since there are almost equal probabilities for the two branches of the DD reaction (Eqs. 12 and 13). However, while some groups have detected heat or neutrons and others have detected tritium or helium, most have obtained null results. It is very important that Pons and Fleischmann release very specific details of their experimental procedure so that this strange effect can be studied and more fully understood.

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The Pons and Fleischmann experiment is a simple electrolysis experiment in which two electrodes are put into an electrolyte consisting of "heavy" water, D_2O, and LiOD, a salt which dissociates into ions and allows the heavy water to conduct electricity between the cathode and the anode. The electric current then forces the dissociation of the D_2O with the end result that oxygen gas is produced at the anode

$$2D_2O \longrightarrow O_2 + 4D^+ + 4e^- \qquad \text{(Ref. 7)} \qquad (18)$$

and that deuterium gas is produced at the cathode.

$$2e^- + 2D_2O \longrightarrow D_2 + 2OD^- \qquad \text{(Ref. 7)} \qquad (19)$$

The cathode, being made of palladium (or titanium), has a very high affinity for the absorbtion of deuterium gas which diffuses into the lattice structure. If we define the ratio of deuterium atoms to palladium ions in the lattice structure to be the loading, x, of the metal, we are left with PdD_x. At STP, palladium can absorb up to 380 times its own volume of deuterium forming a hydride with the non-stoichiometric formula $PdD_{0.6}$. Using other methods such as electrolysis to force more ions into the metal, loadings of 1.0 can be attained. Neutron diffraction has been used to determine that the deuterons occupy the octahedral sites in the palladium lattice. It is proposed that by forcing more than one deuteron into a single lattice site, that there is a dramatic decrease in the equilibrium separation between the deuterons. This would result in a large increase in the tunneling probability of the two particle system because of the decreased barrier width. It was hoped that this could explain the incredible increase in the fusion cross section and lead to the observed fusion rates.

LATTICE EFFECTS ON PENETRABILITIES

In free molecular deuterium, the equilibrium separation is 0.74 A which leads to a calculated fusion reaction rate of about 10^{-70} per D_2 molecule per second (Ref. 9). However, if the deuterons are placed in a lattice, the potential that exists between these particles must now be changed to account for the effects of the lattice electrons. By including the attractive potential of the electrons, the Coulomb barrier is effectively "screened", or decreased, so that the repulsive potential between the deuterons drops off more quickly, which allows for a

greater penetrability and a corresponding increase in the fusion rate. Another possibility is that the electrons have an "effective mass" which may bring the deuterons much closer together like a muon does in muon-catalyzed fusion. In muon-catalyzed fusion, a muon (which is a very large, negatively charged particle with 200 times the mass of an ordinary electron) together with a deuteron and a triton forms a very tightly bound muo-molecule. This muo-molecule results in a dramatic decrease in the DT separation and results in a fusion rate of about 10^{12} fusions per second, an increase of 82 orders of magnitude (Ref. 9). Similarly, if the lattice electrons could have an effective mass of 5 times the normal electron mass, the theoretical fusion rates could be brought into agreement with the results of Jones et. al., but an effective mass of 10 is needed to explain the results of Pons and Fleischmann (Ref. 2). However, no plausible mechanism is currently known which could account for such increases.

Very little is known about fusion reactions at very low energies. It is important to learn about cross sections at high energies and use this information to investigate low energy cross sections. At energies on the order of a few keV's, the DT cross section is almost 3 orders of magnitude larger than DD. Since the reduced mass enters the numerator of the decaying exponential of the barrier penetration factor (see Eq. 6), tunneling is more likely for systems with a smaller reduced mass. This suggests that at some low energy, the cross section for DD is greater than for that of DT (actually both are less than for p+D which has an even smaller reduced mass). However, experimental verification of these numbers is difficult if not impossible. One way to predict cross sections at relatively low energies is by solving the radial s-wave (l=0) wave equation given by

$$\left[-\frac{d^2}{dr^2} + \phi(r) - k^2 \right] U(r) = 0 \tag{20}$$

$$\phi(r) = \frac{2MV(r)}{\hbar^2} \tag{21}$$

$$V(r) = \frac{e^2}{a_0} \frac{e^{-r/a_0}}{1-e^{-r/a_v}} \tag{22}$$

$$k^2 = \frac{2ME}{\hbar^2} \tag{23}$$

where the Hulthen potential is used rather than the pure Coulomb potential due to the screening by the electrons in the metal lattice. The Hulthen potential takes the form of Equation 22 where a_0 is the screening length of the metal. The screening length is a function of electron density and can be found using the Thomas-Fermi model. The screening length is found to be 0.39 Å in palladium and 0.45 Å in titanium (Ref. 10). Figure 1 is a graph of the ratio of the unscreened to the screened potential for the palladium screening length of 0.39 Å.

By solving the wave equation, we are looking to find an analytic formula for the penetrability in a two particle system. The penetrability is a measure of the tunneling probability which can then be related to the cross section. If we look for the regular solution of Equation 20 (i.e., one that goes to zero as r-->0) of the form

$$D(k,r) = Ne^{ikr}(1-e^{-r/a_0})h(k,r) \qquad (24)$$

we get the following hypergeometric equation for h

$$z(1-z)h'' + [2-(a+b+1)z]h' - abh = 0 \qquad (25)$$

with $\quad h' = \dfrac{dh}{dz} \qquad z = 1-e^{-r/a_0}$

$$a = 1 + i\alpha_- \qquad b = 1 - i\alpha_+$$

$$\alpha_{\pm} = ka_0 \left[1 + \frac{2Me^2}{\hbar^2k^2a_0} \right]^{1/2} \pm ka_0 \qquad (26)$$

which when solved gives a formula for the penetrability in the Hulthen potential (Ref. 11),

$$P = \frac{\pi e^2}{\hbar v} \frac{\sinh(2\pi ka_0)}{\sinh(\pi\alpha_+)\,\sinh(\pi\alpha_-)}. \qquad (27)$$

where v is the relative velocity. In the limit that the screening length approaches infinity, the Hulthen potential becomes

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the unscreened Coulomb potential and the penetrability given in Equation 27 approaches the Coulomb penetrability (Ref. 11)

$$P = \frac{\pi e^2 \exp(-\pi e^2/\hbar v)}{\hbar v \ \sinh(\pi e^2/\hbar v)} \tag{28}$$

and in the limit that v-->0, this reduces to

$$P = \frac{2\pi e^2}{\hbar v} \exp{\frac{-2\pi e^2}{\hbar v}} \qquad \text{(Ref. 11)} \tag{29}$$

where the exponential term is the well known Gamow factor (Ref. 12). The Gamow factor gives a very good description of fusion cross sections between free particles at energies on the order of a few keV's. However, in the case of cold fusion, it is necessary to use Equation 27 since there is screening by the lattice electrons. Using this formula, the cross section is found to be

$$\sigma(E) = \frac{K_0 \pi e^2 M}{2\hbar E} \ \frac{\sinh(2\pi ka_0)}{\sinh(\pi\alpha_+) \ \sinh(\pi\alpha_-)} \tag{30}$$

where the energy is in the center of mass frame, and K_0 is the reaction constant. Table 1 shows calculated values for DD and DT cross sections at low energies using the expected palladium screening length. Figure 2 shows that the DD and DT cross sections are equal at about 57 eV. Above this level the DT cross section is higher as is expected from measured values at higher energies. Since the energies of particles in the lattice are expected to be less than 57 eV, the DD reaction should be more likely than DT. At even lower energies, in the neighborhood of 10 eV, the DD reaction is about 10,000 times more likely to occur than the DT reaction (Ref. 3). However, both cross sections are smaller than that of pD which should be the dominant reaction at such low energies because of its smaller reduced mass. However, no evidence of this reaction, which procedes according to

$$p + D \ \text{---}> \ Y + {}^{3}He \qquad \text{(Ref. 4)} \tag{31}$$
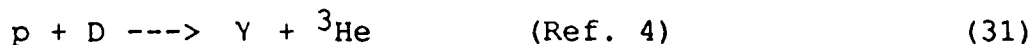
is detected which adds more confusion to this phenomenon. Table 2 shows cross sections for DD, DT and pD for different values of screening length. The screening length is expected to be about 0.4 Å in palladium. If somehow the screening length can be changed, dramatic changes in the fusion cross sections can be

obtained (Ref. 11). Jones et al. have reported fusion rates on the order of 10^{-23} fusions/DD pair/s. If the unit cell of palladium has about 10^{25} DD pairs/cm^3, this implies a fusion rate of 100 fusions/cm^3/s. This would require a DD cross section on the order of 10^{-30} barns. However, if we assume that the deuterons somehow gain a small amount of energy, say $E_{cm} = 10$ eV (this is actually quite a bit of energy since expected vibrational energies inside the lattice are less than 1 eV), the expected cross section for the unscreened Coulomb potential (Eq. 29) is about 10^{-130} barns (Fig. 3 shows the increased penetrability versus screening length, while Figs. 4-6 show the increased penetrability in DD, DT, and pD versus lab energy). This means that the screening must increase the penetrability by a factor of 10^{100}! Using the calculated palladium screening length, the cross section is about 10^{-83} barns, which is still 53 orders of magnitude too small. If we vary the screening length for each energy, we see that the screening length must be decreased by about a factor of 13 (to 0.03 Å) to get cross sections as large as 10^{-30} barns and explain such unexpected fusion rates.

CONCLUSIONS

The results given in this paper, based on the studies of quantum tunneling effects on low energy fusion cross sections, provide a possible mechanism by which low temperature fusion could become possible, i.e., could explain the orders of magnitude necessary to account for recent experimental results. As stated before, no currently known physical phenomenon can explain such decreased screening lengths or effective masses or charges. Further experimental observations of low temperature fusion cross sections are much needed to verify the validity of the Gamow factors of various fuels as described in this report.

TABLE 1

DD, DT, and pD cross sections for various lab energies

$(a_0 = 0.39 \text{ Å})$

E_{lab} (eV)	DD	DT	pD
10	4.21E-96	4.53E-100	2.37E-79
20	2.60E-83	1.60E-85	2.31E-68
30	4.53E-75	2.55E-76	1.76E-61
40	4.89E-69	1.14E-69	1.51E-56
50	2.53E-64	1.60E-64	9.43E-53
60	1.72E-60	2.24E-60	1.05E-49
70	2.78E-57	6.28E-57	3.48E-47
80	1.52E-54	5.31E-54	4.74E-45
90	3.64E-52	1.80E-51	3.26E-43
100	4.50E-50	2.94E-49	1.32E-41
300	4.66E-31	1.62E-29	1.87E-27
500	2.48E-24	1.09E-22	1.29E-22
700	1.32E-20	6.11E-19	5.63E-20
1000	3.22E-17	1.48E-15	1.35E-17
11000	6.57E-05	9.66E-04	2.66E-09
21000	1.82E-03	1.36E-02	1.89E-08

TABLE 2

DD, DT and pD cross sections at $E_{cm} = 10$ eV

for various screening lengths.

a_0 (Å)	DD	DT	pD
0.01	1.39E-17	1.92E-17	2.67E-19
0.02	3.08E-25	1.17E-25	2.37E-25
0.03	9.57E-31	1.57E-31	1.16E-29
0.04	3.73E-35	3.30E-36	4.40E-33
0.05	7.19E-39	3.94E-40	6.06E-36
0.06	4.27E-42	1.60E-43	2.06E-38
0.07	5.91E-45	1.61E-46	1.38E-40
0.08	1.58E-47	3.31E-49	1.56E-42
0.09	7.24E-50	1.21E-51	2.71E-44
0.10	5.17E-52	7.17E-54	6.68E-46
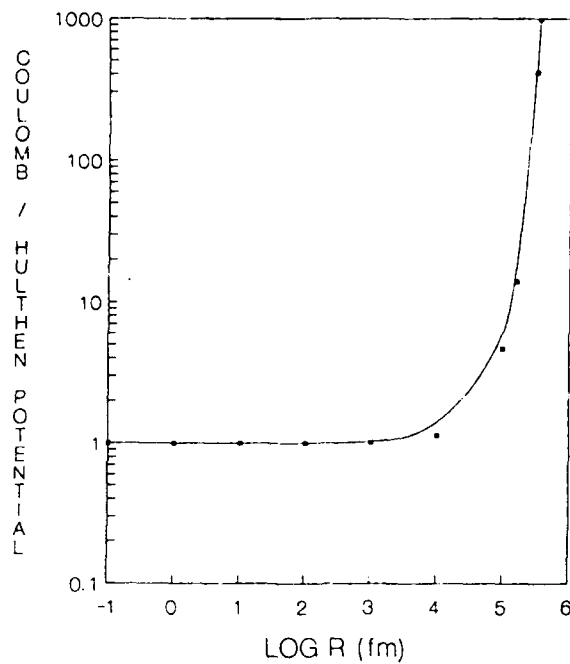
Figure 1

Ratio of Unscreened to Screened Coulomb Potential
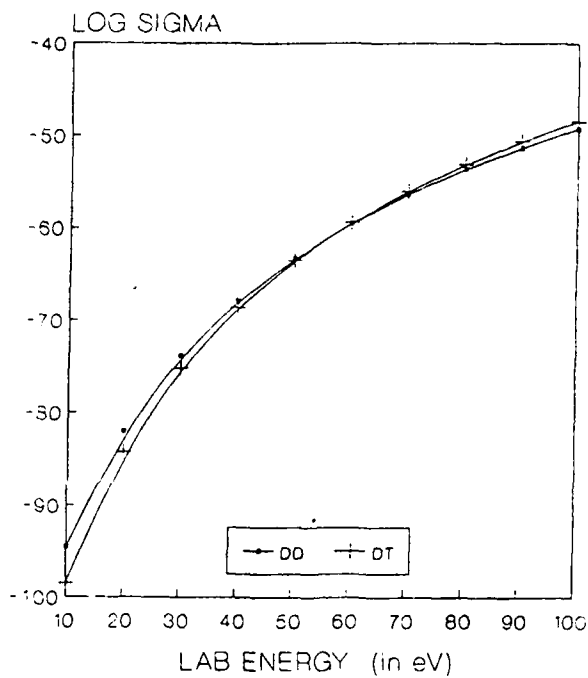
Figure 2

Cross Sections for DD and DT vs Lab Energy
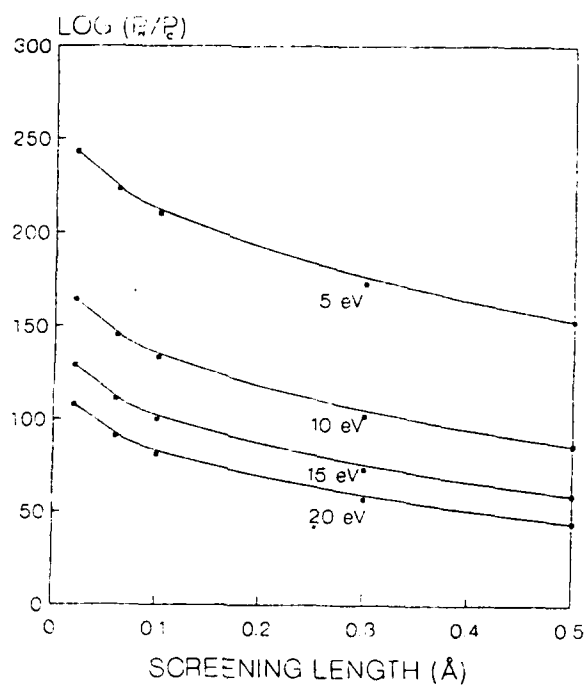(for DT, only the D induced reaction is included)

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Figure 3

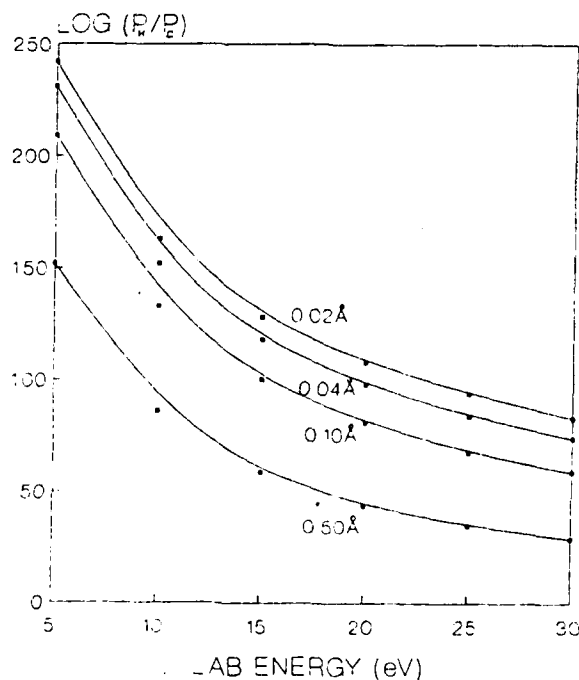Increased Penetrability in DD versus
Screening Length (for various lab energies)

Figure 4

Increased Penetrabilty versus
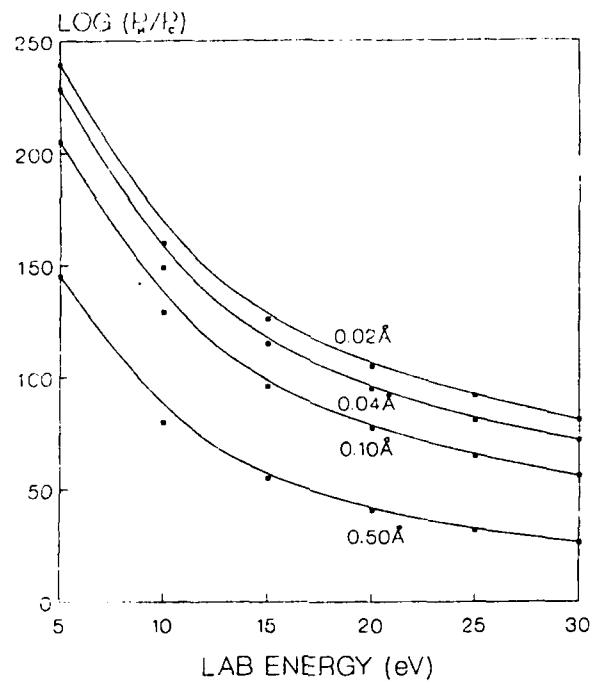Lab Energy (for various screening lengths)

14

LOG (P/P)

Figure 5

Increased Penetrability in DT versus
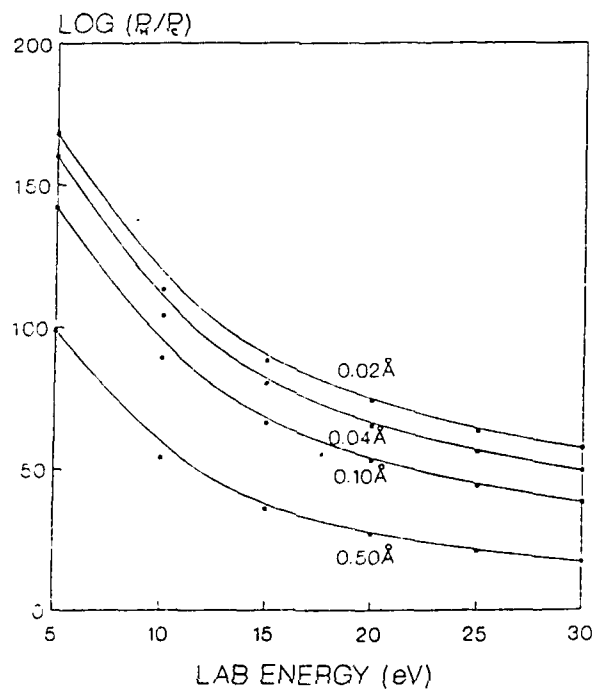Lab Energies (for various screening lengths)

LOG (P/P)

Figure 6

Increased Penetrability in pD versus
Lab Energy (for various screening lengths)

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